Analytical contradictions of the 'fixed - node' density matrices

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Over the last decades the 'fixed-node method' has been widely used for a numerical treatment of thermodynamic properties of strongly correlated Fermi systems. In this work correctness of the 'fixed -node method' for ideal Fermi systems has been analytically analyzed. Rigorous consideration shows that the 'fixed-node' calculation of the density matrix even for two ideal fermions leads to contradictions. Analogous contradictions results from the virial decomposition of the many fermion 'fixed – node' density. Numerical results of the 'direct path integral Monte Carlo simulations' show that the 'fixed – node method' describes the thermodynamic properties of the strongly coupled fermions rather well only at weak degeneracy. Difference in results obtained by these methods increases systematically with the growth of the degeneracy at high density and low temperatures. The reason of this difference results from the replacement of the initial condition by the zero boundary conditions for the density matrix in the Bloch equation in the 'fixed-node approach'. This replacement results in uncontrolled errors in calculations of thermodynamic quantities due to the wrong description of statistical effects. The main conclusion of this work is that the 'fixed-node method' can not reproduce density matrices of fermions and should be considered as uncontrolled empirical approach in treatment of thermodynamics of Fermi systems.

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I. INTRODUCTION

Over the last decades significant progress has been observed in theoretical studies of thermodynamic properties of strongly correlated systems of fermions at non-zero temperatures, which is mainly conditioned by the application of numerical simulations (see review [1]). The reason for this success is the possibility of an explicit representation of the low-temperature density matrix in the form of a finite-dimensional approximation of the Wiener path integrals [2] without any preliminary physical approximations, which require some physical parameters to be small. The main difficulty for path integral Monte Carlo studies (PIMC) of Fermi systems results from the requirement of antisymmetrization of the density matrix in the partition function [2]. As a result all thermodynamic quantities are presented as the sum of alternating sign terms related to even and odd permutations of particles. So the thermodynamic quantities are determined by the small difference of two large numbers, which are the sums of positive and negative terms. The numerical calculation in this case is severely hampered. This difficulty is known in the literature as the 'sign problem'. To overcome this issue some approaches have been developed, among which the 'fixed-node method' [1, 3–5] is widely known.

The main idea of the 'fixed-node method' [1, 3–5] consists in replacement of initial condition by zero boundary conditions for Bloch equation describing fermion density matrices. So instead of initial condition the 'fixed-node' density matrix is to take the 'zero conditions' on the boundaries of the domain of the positive values of an additional 'trial antisymmetric density matrix' presented in the form of path integral.

The purpose of this work is to give an analytical proof that this replacement results in contradictions in explicit calculations of the density matrix even for two ideal fermions. The analogous conclusion have been analytically obtained twelve years ago in [6] from virial decomposition of the many fermion 'fixed-node' density matrix'. However paper [6] is very difficult for understanding as used the Rueele algebraic approach [7] and was missed by the scientific community. This is the reason to discuss correctness of the 'fixed - node method' once more using more simple mathematical technique. The main result of this work and paper [6] is that the 'fixed–node method' should be considered as an ***uncontrolled*** empirical approach in treatment of thermodynamics of fermions.

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II. DENSITY MATRIX BY THE 'FIXED - NODE METHOD'

Thermodynamic properties of the fermion quantum system at non-zero temperature are defined by the appropriate derivatives of the logarithm of the partition function $Q_N = Tr\{\rho\}$. Here $\rho = \exp(-\beta\hat{H})$ is the density matrix of a quantum system of particles with the Hamiltonian $\hat{H} = \hat{K} + \hat{U}$ equal to the sum of kinetic $\hat{K}$ and potential energy $\hat{U}$ operators, while $\beta = 1/k_B T$. For our purposes it is enough to consider one dimensional (1D) system of two ideal fermions, so $\hat{U} \equiv 0$, while the kinetic energy operator is the sum of two kinetic energy operators related to each particle $\hat{K} = \hat{K_1} + \hat{K_2}$. Density matrix is the solution of the operator Bloch equation

$$\frac{\partial\hat{\rho}}{\partial\beta} = -\hat{K}\hat{\rho} \tag{1}$$

with the initial condition $\hat{\rho}|_{\beta=0} = \hat{1}$.

This operator equation in coordinate representation for fermions can be written in the form [3, 4]

$$\frac{\partial\rho_F(R,R_0;\beta)}{\partial\beta} = -\hat{K}(R)\rho_F(R,R_0;\beta) \tag{2}$$

with the initial condition

$$\rho_F(R,R_0;0) = \sum_P (-1)^{\kappa P}\delta(R - PR_0) \tag{3}$$

where R is the set of coordinates of all particles. One of the possible coordinate representation of the fermion density matrix looks like

$$\rho_F(R,R_0;\beta) = \sum_\alpha \exp(-\beta E_\alpha)\phi^*_\alpha(R)\phi_\alpha(R_0) \tag{4}$$

where the sum is over the complete set of antisymmetric eigenfunctions $\phi_\alpha(R)$ of $\hat{H}$.

Another ***exact*** popular coordinate representation of operator $\hat{\rho}$ follows from the operator identity $e^{-\beta\hat{K}} \equiv e^{-\Delta\beta\hat{K}}\cdots e^{-\Delta\beta\hat{K}}\ldots e^{-\Delta\beta\hat{K}}$ ***for any (even of oder unity) integer fixed*** M. Here the r.h.s. contains M identical factors with $\Delta\beta = \beta/M$. So one can ***exactly*** present the ideal density matrix in the form of finite– difference expression of the path integral

$$\rho_F(R_M,R_0;\beta) = \frac{1}{N!}\sum_P (-1)^{\kappa_P}\int dR_1\cdots dR_{M-1}\left(\prod_{k=1}^{M-1}\rho(R_{k-1},R_k;\Delta\beta)\right)\rho(R_{M-1},PR_M;\Delta\beta) \tag{5}$$

where N is the number of fermions. For $N = 2$ arguments are two dimensional (2D) vectors composed by the coordinates of the first and second particle on $1D$ axes $X^{(1)}$ and $X^{(2)}$ and $\rho(R_{k-1},R_k;\Delta\beta)$ are distinguishable particle density matrices. Antisymmetry is put in by the antisymmetrization. The sum runs over all permutations with parity κ_P acting on indexes of particles. These density matrices are functions of the 2D arguments R_M, R_0 on $(X^{(1)}, X^{(2)})$ plane and inverse temperature β.

Mathematical meaning of expression (5) for density matrix of two particles is illustrated by Fig. 1, where vectors R_k are presented by circles (called often as 'beads'), while density matrices $\rho(R_{k-1},R_k;\Delta\beta)$ are denoted by segments of lines. Sometimes instead of coordinate $\left\{X_k^{(1)}, X_k^{(2)}\right\}$ it is convenient to use coordinates $\{\gamma_k,\eta_k\}$ defined by expressions $\gamma_k = 0.5\left(X_k^{(1)} + X_k^{(2)}\right)$ and $\eta_k = \left(X_k^{(1)} - X_k^{(2)}\right)$, so $R_k = \left\{X_k^{(1)}, X_k^{(2)}\right\} = \{\gamma_k,\eta_k\}$. Modulus of Jacobian related to the change of variables of integration in Eq. (5) from the system of coordinates $\left\{X_k^{(1)}, X_k^{(2)}\right\}$ to the system $\{\gamma_k,\eta_k\}$ is equal to unity. Action of perturbation P is illustrated in Fig. 1 by the arrow with letter P (see Fig. 1). For two fermions the sum over permutations is reduced to the sum of contributions of identical and non identical permutations with opposite signs. The density matrix has the following general properties:

$$\rho_F(R,R_0;\beta) = \rho_F(R_0,R;\beta) = (-1)^{\kappa P}\rho_F(PR,R_0;\beta) \tag{6}$$

For further comparisons with the 'fixed - node' density matrix let us remind the solution of the Bloch equation (2) with the initial condition (3). Density matrices in (5) are well known for ideal particles and can be written in the form [2] :

$$\rho(R_{k-1},R_k;\Delta\beta) = \frac{\exp\left(-\frac{\pi|R_k-R_{k-1}|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}^2} = \frac{\exp\left(-\frac{2\pi|\gamma_k-\gamma_{k-1}|^2}{\tilde{\lambda}^2}\right)\exp\left(-\frac{\pi|\eta_k-\eta_{k-1}|^2}{2\tilde{\lambda}^2}\right)}{\tilde{\lambda}^2} \tag{7}$$

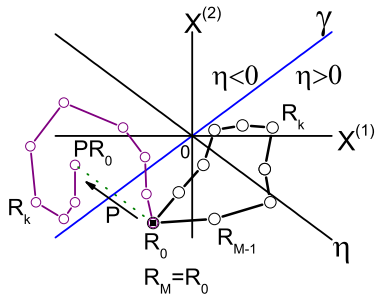

FIG. 1: (Color online) Configurational space of two free fermions. Plotted are the paths related to the two possible permutations: identical (below line γ) and non-identical (crossing line γ) permutations.

where $\tilde{\lambda}^2 = 2\pi\hbar^2\Delta\beta/m$ is the thermal wave length related to $\Delta\beta$. The last factor in (5) for permutation P has the form

$$\rho(R_{M-1}, PR_M; \Delta\beta) = \frac{\exp\left(-\frac{\pi|PR_M - R_{M-1}|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}^2} = \frac{\exp\left(-\frac{2\pi|P\gamma_M - \gamma_{M-1}|^2}{\tilde{\lambda}^2}\right)\exp\left(-\frac{\pi|P\eta_M - \eta_{M-1}|^2}{2\tilde{\lambda}^2}\right)}{\tilde{\lambda}^2}. \tag{8}$$

So the exact well known expression for two particle antisymmetrized density matrix looks like [2]

$$\begin{aligned}\rho_F(R_M, R_0; \beta) &= \frac{1}{2}\int dR_1 \cdots dR_{M-1}\left(\prod_{k=1}^{M-1}\frac{\exp\left(-\frac{\pi|R_k - R_{k-1}|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}^2}\right)\frac{\exp\left(-\frac{2\pi|\gamma_M - \gamma_{M-1}|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}} \\ &\times\left\{\frac{\exp\left(-\frac{\pi|\eta_M - \eta_{M-1}|^2}{2\tilde{\lambda}^2}\right) - \exp\left(-\frac{\pi|P\eta_M - \eta_{M-1}|^2}{2\tilde{\lambda}^2}\right)}{\tilde{\lambda}}\right\} \\ &\equiv \frac{1}{2}\frac{\exp\left(-\frac{2\pi|\gamma_M - \gamma_0|^2}{\lambda^2}\right)}{\lambda}\left\{\frac{\exp\left(-\frac{\pi|\eta_M - \eta_0|^2}{2\lambda^2}\right) - \exp\left(-\frac{\pi|P\eta_M - \eta_0|^2}{2\lambda^2}\right)}{\lambda}\right\}\end{aligned} \tag{9}$$

with $\lambda^2 = 2\pi\hbar^2\beta/m$, $P\gamma_M = \gamma_M$ and $P\eta_M = -\eta_M$. If $\{\gamma_M, \eta_M\} = \{\gamma_0, \eta_0\}$ then $P\gamma_M = \gamma_0$ and $P\eta_M = -\eta_0$ (see Fig. 1).

Now let us consider the basic statements of the 'fixed - node method'. The authors of [3, 4] denote the second argument R_0 of the density matrix as the ***'reference point'*** and ***'the set of points*** R_t ***for which there exists a continuous 'space–imaginary time' path with*** $\rho_F(R, R_0; t') > 0$ ***for*** $0 \le t' \le \beta$ ***the reach of*** R_0 ***or*** $\Gamma(R_0, \beta)$***'***. For two ideal fermions the reach can be analytically obtained [3, 4]. As example the reach (the half plane $\eta > 0$) for $\eta_0 > 0$ is shown in Fig. 1. The reach does not depend on temperature.

The first wrong basic statement of the papers [3, 4] claims that initial condition (3) can be replaced by a ***zero boundary condition on the surface of the reach***. Papers [3, 4] claims that ***'it follows because the fermion density matrix is a unique solution to the Bloch equation (2) with the zero boundary conditions (see Appendix C)'***. However the Bloch equation (2) with the zero boundary conditions is linear equation and, besides the trivial solution identically equal to zero, has an infinite number of solutions distinguishing by constant factors, while the Bloch equation (2) with initial condition (3) has really a unique solution.

Now let us consider general 'fixed – node' solutions of the Bloch equation in the $\gamma - \eta$ plane (see Fig. 1). The authors of [3, 4] claimed that to obtain the 'fixed – node' density matrix ***'one simply restricts the paths in Eq. (5) to lie in the*** $\Gamma(R_0, \beta)$***'***. This means that restriction of integration over $R_1, \cdots, R_{M-1}$ in (5) ***by the reach*** gives the exact solution of Eq. (2) with initial condition (3). The fallaciousness of this statement can be easily proved by explicit integration over variables $R_1, \cdots, R_{M-1}$ in the reach for 1D two ideal fermions for $M = 2$ as well as for arbitrary integer M. The boundary surface of the 2D reach for two ideal fermions is exactly known and according to papers [3, 4] is the line $\eta = 0$ in Fig. 1. So on the whole $(X^{(1)}, X^{(2)})$ plane the 'fixed–node' general solution of Eq. (2) looks like (for two ideal fermions)

$$\rho_F(R_M, R_0; \beta) = \frac{C_1}{2}\int dR_1 \cdots dR_{M-1}\left(\prod_{k=1}^{M-1}\frac{\exp\left(-\frac{\pi|R_k - R_{k-1}|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}^2}\right)\frac{\exp\left(-\frac{2\pi|\gamma_M - \gamma_{M-1}|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}}$$

$$\times\left\{\frac{\exp\left(-\frac{\pi|\eta_M-\eta_{M-1}|^2}{2\tilde{\lambda}^2}\right)-\exp\left(-\frac{\pi|P\eta_M-\eta_{M-1}|^2}{2\tilde{\lambda}^2}\right)}{\tilde{\lambda}}\right\}\theta(\eta_0)\theta(\eta_1)\cdots\theta(\eta_M)$$

$$+\frac{C_2}{2}\int dR_1\cdots dR_{M-1}\left(\prod_{k=1}^{M-1}\frac{\exp\left(-\frac{\pi|R_k-R_{k-1}|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}^2}\right)\frac{\exp\left(-\frac{2\pi|\gamma_M-\gamma_{M-1}|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}}$$

$$\times\left\{\frac{\exp\left(-\frac{\pi|\eta_M-\eta_{M-1}|^2}{2\tilde{\lambda}^2}\right)-\exp\left(-\frac{\pi|P\eta_M-\eta_{M-1}|^2}{2\tilde{\lambda}^2}\right)}{\tilde{\lambda}}\right\}\theta(-\eta_0)\theta(-\eta_1)\cdots\theta(-\eta_M), \tag{10}$$

where $\theta(\eta)$ is the theta function equal to zero for $\eta<0$ and equal to unity in the opposite case $\eta\geq 0$. The theta functions restrict to the reach the domains of integration. Now assume that all 'basic statements' of papers [3, 4] are ***correct***. Then using the mentioned above general properties of the density matrix we have to admit that integration over $R_2\cdots,R_{M-1}$ in the reach gives the exact solution of Eq. (2) with initial condition (3). So the density matrix in the 'fixed–node method' (10) can be transformed to the following integral over the last variable R_1:

$$\rho_F(R_M,R_0;\beta)=\frac{1}{2}\int dR_1\frac{\exp\left(-\frac{\pi|R_1-R_0|^2}{\tilde{\lambda}^2}\right)}{\tilde{\lambda}^2}\frac{\exp\left(-\frac{2\pi|\gamma_M-\gamma_1|^2}{(M-1)\tilde{\lambda}^2}\right)}{\sqrt{(M-1)}\tilde{\lambda}} \tag{11}$$

$$\times[C_1\frac{\exp\left(-\frac{\pi|\eta_M-\eta_1|^2}{2(M-1)\tilde{\lambda}^2}\right)-\exp\left(-\frac{\pi|P\eta_M-\eta_1|^2}{2(M-1)\tilde{\lambda}^2}\right)}{\sqrt{(M-1)}\tilde{\lambda}}\theta(\eta_0)\theta(\eta_1)\theta(\eta_M)$$

$$+C_2\frac{\exp\left(-\frac{\pi|\eta_M-\eta_1|^2}{2(M-1)\tilde{\lambda}^2}\right)-\exp\left(-\frac{\pi|P\eta_M-\eta_1|^2}{2(M-1)\tilde{\lambda}^2}\right)}{\sqrt{(M-1)}\tilde{\lambda}}\theta(-\eta_0)\theta(-\eta_1)\theta(-\eta_M)]=\frac{1}{2}\frac{\exp\left(-\frac{2\pi|\gamma_M-\gamma_0|^2}{\lambda^2}\right)}{2\lambda}$$

$$\times[C_1\theta(\eta_0)\theta(\eta_M)\frac{\exp\left(-\frac{\pi|\eta_M-\eta_0|^2}{2\lambda^2}\right)erfc\left(-\sqrt{\pi}\frac{(M-1)\eta_0+\eta_M}{\sqrt{2M(M-1)}\tilde{\lambda}}\right)-\exp\left(-\frac{\pi|P\eta_M-\eta_0|^2}{2\lambda^2}\right)erfc\left(-\sqrt{\pi}\frac{(M-1)\eta_0+P\eta_M}{\sqrt{2M(M-1)}\tilde{\lambda}}\right)}{\lambda}$$

$$+C_2\theta(-\eta_0)\theta(-\eta_M)\frac{\exp\left(-\frac{\pi|\eta_M-\eta_0|^2}{2\lambda^2}\right)erfc\left(-\sqrt{\pi}\frac{-(M-1)\eta_0+\eta_M}{\sqrt{2M(M-1)}\tilde{\lambda}}\right)-\exp\left(-\frac{\pi|P\eta_M-\eta_0|^2}{2\lambda^2}\right)erfc\left(-\sqrt{\pi}\frac{-(M-1)\eta_0+P\eta_M}{\sqrt{2M(M-1)}\tilde{\lambda}}\right)}{\lambda}]$$

Thus instead of the exact density matrix (9) we have infinite number of the 'fixed – node' density matrices (11). These density matrices take the 'zero boundary conditions' on the surface of the reach ($\eta_M=0$) for any $M\geq 2$, but depend on two arbitrary constants. More over they depend on complementary error functions. (11) is correct for any fixed $M\geq 2$.

For further detail analysis of the function (11) let us consider the limit of $\Delta\beta\to 0$ ($M\to\infty$). Using definition of complementary error functions one can transform (11) to the form:

$$\rho_F(R_M,R_0;\beta)=\frac{\exp\left(-\frac{2\pi|\gamma_M-\gamma_0|^2}{\lambda^2}\right)}{4\lambda}$$

$$\times[C_1\theta(\eta_M)\frac{(\exp\left(-\frac{\pi|\eta_M-\eta_0|^2}{2\lambda^2}\right)-\exp\left(-\frac{\pi|P\eta_M-\eta_0|^2}{2\lambda^2}\right))(1+sign(\eta_0))}{\lambda}$$

$$+C_2\theta(-\eta_M)\frac{(\exp\left(-\frac{\pi|\eta_M-\eta_0|^2}{2\lambda^2}\right)-\exp\left(-\frac{\pi|P\eta_M-\eta_0|^2}{2\lambda^2}\right))(1-sign(\eta_0))}{\lambda}] \tag{12}$$

where

$$lim_{\Delta\beta\to 0}erfc\left(-\sqrt{\pi}\frac{\pm(M-1)\eta_0+P\eta_M}{\sqrt{2M(M-1)}\tilde{\lambda}}\right)=1-lim_{\Delta\beta\to 0}erf\left(-\sqrt{\pi}\frac{\pm(M-1)\eta_0+P\eta_M}{\sqrt{2M(M-1)}\tilde{\lambda}}\right)=1\pm sign(\eta_0) \tag{13}$$

and erf is the error function. Here $sign(\eta_0)$ is equal to plus unity for $\eta_0>0$ and minus unity for $\eta_0<0$.

One can easily see from (12) that in the limit $\Delta\beta\to 0$ the 'fixed–node' density matrix for two arbitrary constants (C_1 and C_2) takes the 'zero boundary conditions' on the surface of the reach (for $\eta_M=0$). The 'fix-node' density matrix (12) differs from exact expressions Eq. (9) and contrary to it is ***a non analytical function***. More over the

'fix-node' density matrix (12) is identically equal to zero if η_0 and η_M are lying in opposite half planes ($\eta > 0$ and $\eta < 0$) of the $\gamma - \eta$ plane, while this is not the case for exact density matrix (9). All these contradictions mean that the integration in the reach can not reproduce the exact solution of Eq. (2) with initial condition (3) in spite of the 'second basic statement' of papers [3, 4].

An alternative approach for studies Fermi systems without replacement of initial conditions by zero boundary conditions for the Bloch equation is known in literature as the direct path integral Monte Carlo simulation (DPIMC) [6, 8–11]. In this approach the sum over all permutations is represented identically as a determinant, which can be exactly calculated by the direct methods of linear algebra. The accuracy of this approach depends only on the errors of the finite-dimensional approximations of the path integrals and can be improved systematically. Comparison with results of the DPIMC simulation show that the fixed – node method describes the thermodynamic properties of the **strongly coupling** fermions rather well at weak degeneracy, when the main contribution to the partition function comes from the identical permutation [6, 10, 11]. The difference in obtained results increases systematically with the growth of the degeneracy at high density and low temperatures [6, 10, 11]. The reason of this difference is in the replacement of initial condition by the zero boundary conditions for Bloch equation. This replacement results in uncontrolled errors in calculations of thermodynamic quantities due to the wrong description of statistical effects in the system of degenerate interacting and non interacting fermions .

Conclusion.

The 'fixed - node method' can not reproduce correctly even the two fermions density matrix. Analogous conclusion for the many particle density matrix of ideal Fermi system have been analytically obtained in [6] from virial decomposition. So the 'fixed - node method' can not correctly describe the degenerate Fermi systems. The main result of this simple work and paper [6] is that the 'fixed - node method' should be considered as ***uncontrolled*** empirical approach in treatment of thermodynamics of degenerate non interacting fermions. Numerical simulations of thermodynamic quantities for interacting fermions by the direct path integral Monte Carlo method results in analogous conclusions.

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